n-ELECTRON ($n=2, 4, 6, 8$) SINGLETS AS S^2 EIGENFUNCTIONS

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(Received June 1, 1974)

n-electron ($n=2, 4, 6, 8$) singlets as S^2 eigenfunctions were constructed by the method of spin operators.

Introduction

Only for certain rather special forms of the potential function is the wave equation completely soluble in closed terms; in general, different approximate methods must be applied. The most important one of these methods is the general method of configuration interaction. In the investigation of molecules by configuration interaction one is usually faced with the problem of setting up the states of definite multiplicity for the various configurations. If the states of the various configurations are described by Slater determinants, the linear combination of Slater determinants can be regarded as the best zero-order eigenfunction. Then, the energy, to first order, is given by the roots of the usual secular equation. The secular determinant can be broken down into a product of determinants of lower order by means of the operators S^2 and S_z. A simple and direct method to construct the suitable eigenfunctions for an n-electron system, fulfilling the operator equation of both operators S^2 and S_z simultaneously, was suggested in former papers [1—3]. This paper presents a brief discussion of the proposed operator technique developed for the problem of n-electron ($n=2, 4, 6, 8$) singlets.

The spin operator

It is well known that the number of independent spin states is in fact [4]

$$N(s) = \binom{n}{\frac{1}{2}n-s} - \binom{n}{\frac{1}{2}n-s-1}.$$

This result may be justified by using the so-called branching diagram, a pictorial description of adding the spin angular momenta of electrons one by one (Fig. 1).

As can be seen, the branching diagram not only shows how many states of a given multiplicity there are for the n-electrons, but application of the methods of vector addition to the angular momentum immediately shows how the states are actually constructed.

The method suggested for the construction of the S^2 eigenfunction is nothing else than the abstract formulation of the method of branching diagrams. If one unites the part systems $X_1, X_2, X_3, \ldots, X_{2n-1}, X_{2n}$, containing x_1 electrons with

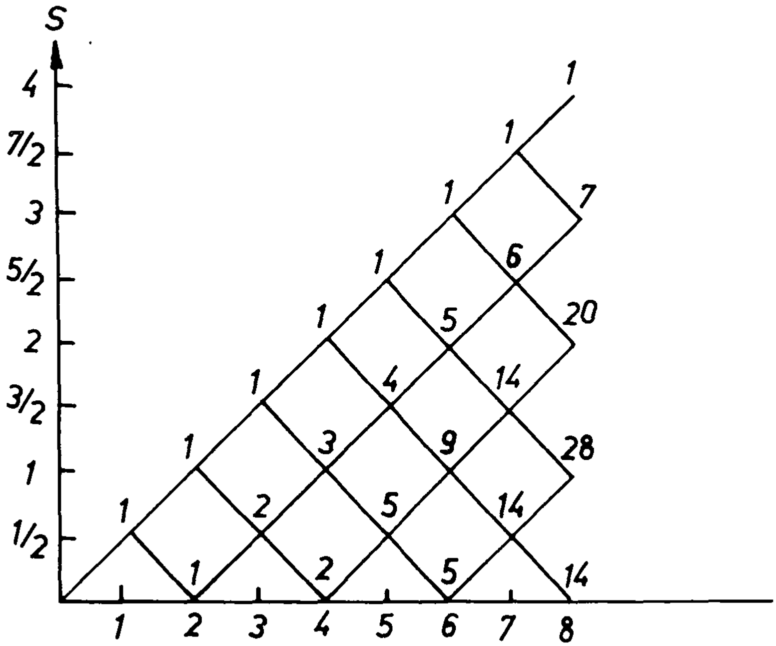

Fig. 1

parallel spin α, x_2 electrons with parallel spin β, x_3 electrons with parallel spin $\alpha, \ldots, x_{2n-1}$ electrons with parallel spin α and x_{2n} electron with parallel spin β, to a system $X_1 X_2 X_3 \ldots X_{2n-1} X_{2n}$ with the resulting spin $\frac{x_1}{2} - \frac{x_2}{2} + \frac{x_3}{2} - \ldots + \frac{x_{2n-1}}{2} - \frac{x_{2n}}{2}$, then the spin operator which, when operating on the eigenfunctions of the total S_z operator related to maximal projections of total spin, creates each given-function of the total S^2 corresponding to its different eigenvalues, has according to [2], (3. 10) the following form:

$$O_{x_1 x_2 x_3 \ldots x_{2n-1} x_{2n}} = \left(\frac{x_1 - x_2 + x_3 - \ldots + x_{2n-1} - x_{2n} + 1}{x_1 - x_2 + x_3 - \ldots + x_{2n-1} + 1}\right)^{1/2} \times$$

$$\times \left(\frac{x_1 - x_2 + x_3 - \ldots x_{2n-3} - x_{2n-2} + 1}{x_1 - x_2 + x_3 - \ldots x_{2n-3} + 1}\right)^{1/2} \times \ldots \times \left(\frac{x_1 - x_2 + 1}{x_1 + 1}\right)^{1/2} \times$$

$$\times \sum_{k=0}^{x_{2n}} (-1)^k \frac{(x_1-x_2+x_3-\ldots+x_{2n-1}-k)!}{(x_1-x_2+x_3-\ldots+x_{2n-1})!\,k!} (S^-_{X_1X_2X_3\ldots X_{2n-1}} S^+_{X_{2n}})^k \times$$

$$\times \sum_{j=0}^{x_{2n-2}} (-1)^j \frac{(x_1-x_2+x_3-\ldots+x_{2n-3}-j)!}{(x_1-x_2+x_3-\ldots+x_{2n-3})!\,j!} (S^-_{X_1X_2X_3\ldots X_{2n-3}} S^+_{X_{2n-2}})^j \times$$

$$\times \ldots \times \sum_{i=0}^{x_2} \frac{(x_1-i)!}{x_1!\,i!} (S^-_{X_1} S^+_{X_2})^i.$$

The n-electron singlets

Let us denote the Slater determinants describeing the states of n-electron systems as follows:

$n = 2$

$A_1 = |\alpha\beta|, \quad \bar{A}_1 = |\beta\alpha|;$

$n = 4$

$B_1 = |\alpha\alpha\beta\beta|, \quad B_2 = |\alpha\beta\beta\alpha|, \quad B_3 = |\alpha\beta\alpha\beta|; \quad \bar{B}_i = B_i(\alpha \leftrightarrow \beta); \quad B_i^* = B_i + \bar{B}_i;$

$n = 6$

$C_1 = |\alpha\alpha\alpha\beta\beta\beta|, \quad C_2 = |\alpha\alpha\beta\beta\beta\alpha|, \quad C_3 = |\alpha\alpha\beta\beta\alpha\beta|, \quad C_4 = |\alpha\alpha\beta\alpha\beta\beta|,$

$C_5 = |\alpha\beta\beta\beta\alpha\alpha|, \quad C_6 = |\alpha\beta\beta\alpha\alpha\beta|, \quad C_7 = |\alpha\beta\beta\alpha\beta\alpha|, \quad C_8 = |\alpha\beta\alpha\alpha\beta\beta|,$

$C_9 = |\alpha\beta\alpha\beta\beta\alpha|, \quad C_{10} = |\alpha\beta\alpha\beta\alpha\beta|, \quad \bar{C}_i = C_i(\alpha \leftrightarrow \beta), \quad C_i^* = C_i + \bar{C}_i;$

$n = 8$

$D_1 = |\alpha\alpha\alpha\alpha\beta\beta\beta\beta|, \quad D_2 = |\alpha\alpha\alpha\beta\alpha\beta\beta\beta|, \quad D_3 = |\alpha\alpha\alpha\beta\beta\beta\beta\alpha|, \quad D_4 = |\alpha\alpha\alpha\beta\beta\alpha\beta\beta|,$

$D_5 = |\alpha\alpha\alpha\beta\beta\beta\alpha\beta|, \quad D_6 = |\alpha\alpha\beta\alpha\alpha\beta\beta\beta|, \quad D_7 = |\alpha\alpha\beta\alpha\beta\alpha\beta\beta|, \quad D_8 = |\alpha\alpha\beta\alpha\beta\beta\alpha\beta|,$

$D_9 = |\alpha\alpha\beta\alpha\beta\beta\beta\alpha|, \quad D_{10} = |\alpha\alpha\beta\beta\alpha\alpha\beta\beta|, \quad D_{11} = |\alpha\alpha\beta\beta\alpha\beta\alpha\beta|, \quad D_{12} = |\alpha\alpha\beta\beta\alpha\beta\beta\alpha|,$

$D_{13} = |\alpha\alpha\beta\beta\beta\alpha\alpha\beta|, \quad D_{14} = |\alpha\alpha\beta\beta\beta\alpha\beta\alpha|, \quad D_{15} = |\alpha\alpha\beta\beta\beta\beta\alpha\alpha|, \quad D_{16} = |\alpha\beta\beta\beta\beta\alpha\alpha\alpha|,$

$D_{17} = |\alpha\beta\beta\beta\alpha\beta\alpha\alpha|, \quad D_{18} = |\alpha\beta\beta\beta\alpha\alpha\beta\alpha|, \quad D_{19} = |\alpha\beta\beta\beta\alpha\alpha\alpha\beta|, \quad D_{20} = |\alpha\beta\beta\alpha\alpha\alpha\beta\beta|,$

$D_{21} = |\alpha\beta\beta\alpha\alpha\beta\alpha\beta|, \quad D_{22} = |\alpha\beta\beta\alpha\alpha\beta\beta\alpha|, \quad D_{23} = |\alpha\beta\beta\alpha\beta\alpha\alpha\beta|, \quad D_{24} = |\alpha\beta\beta\alpha\beta\alpha\beta\alpha|,$

$D_{25} = |\alpha\beta\beta\alpha\beta\beta\alpha\alpha|, \quad D_{26} = |\alpha\beta\alpha\alpha\alpha\beta\beta\beta|, \quad D_{27} = |\alpha\beta\alpha\alpha\beta\alpha\beta\beta|, \quad D_{28} = |\alpha\beta\alpha\alpha\beta\beta\alpha\beta|,$

$D_{29} = |\alpha\beta\alpha\alpha\beta\beta\beta\alpha|, \quad D_{30} = |\alpha\beta\alpha\beta\alpha\alpha\beta\beta|, \quad D_{31} = |\alpha\beta\alpha\beta\alpha\beta\alpha\beta|, \quad D_{32} = |\alpha\beta\alpha\beta\alpha\beta\beta\alpha|,$

$D_{33} = |\alpha\beta\alpha\beta\beta\alpha\alpha\beta|, \quad D_{34} = |\alpha\beta\alpha\beta\beta\alpha\beta\alpha|, \quad D_{35} = |\alpha\beta\alpha\beta\beta\beta\alpha\alpha|, \quad \bar{D}_i = D_i(\alpha \leftrightarrow \beta),$

$D_i^* = D_i + \bar{D}_i.$

The relating eigenfunctions are as follows:

$$n = 2$$

$$\Phi_1^2 = O_{X_1 X_2} A_1 = \frac{1}{\sqrt{2}}(A_1 - \bar{A}_1);$$

$$n = 4$$

$$\Phi_1^4 = O_{X_1 X_2} B_1 = \frac{1}{\sqrt{3}}\left[B_1^* - \frac{1}{2}(B_2^* + B_3^*)\right],$$

$$\Phi_2^4 = O_{X_1 \dots X_4} B_3 = \frac{1}{2}(B_3^* - B_2^*);$$

$$n = 6$$

$$\Phi_1^6 = O_{X_1 X_2} C_1 = \frac{1}{6}[3(C_1 - \bar{C}_1) + \bar{C}_2 + \bar{C}_3 + \bar{C}_4 + C_5 + C_6 + C_7 + \bar{C}_8 + \bar{C}_9 + \bar{C}_{10} -$$

$$- (C_2 + C_3 + C_4 + \bar{C}_5 + \bar{C}_6 + \bar{C}_7 + C_8 + C_9 + C_{10})],$$

$$\Phi_2^6 = O_{X_1 \dots X_4} C_4 = \frac{1}{2\sqrt{6}}[2(\bar{C}_2 + C_3) - 2(C_2 + \bar{C}_3) + (\bar{C}_6 + C_7 + C_9 + \bar{C}_{10}) -$$

$$- (C_6 + \bar{C}_7 + \bar{C}_9 + C_{10})],$$

$$\Phi_3^6 = O_{X_1 \dots X_4} C_5 = \frac{1}{6\sqrt{2}}[4(C_4 - \bar{C}_4) + 2(\bar{C}_2 + \bar{C}_3 + C_5 + \bar{C}_8) - 2(C_2 + C_3 + \bar{C}_5 + C_8) +$$

$$+ (\bar{C}_6 + \bar{C}_7 + C_9 + C_{10}) - (C_6 + C_7 + \bar{C}_9 + \bar{C}_{10})],$$

$$\Phi_4^6 = O_{X_1 \dots X_4} C_6 = \frac{1}{2\sqrt{6}}[2(C_5 + C_8) - 2(\bar{C}_5 + \bar{C}_8) + (\bar{C}_6 + \bar{C}_7 + \bar{C}_9 + \bar{C}_{10}) -$$

$$- (C_6 + C_7 + C_9 + C_{10})],$$

$$\Phi_5^6 = O_{X_1 \dots X_6} C_{10} = \frac{1}{2\sqrt{2}}[\bar{C}_6 + C_7 + \bar{C}_9 + C_{10} - (C_6 + \bar{C}_7 + C_9 + \bar{C}_{10})];$$

$$n = 8$$

$$\Phi_1^8 = O_{X_1 X_2} D_1 = \frac{\sqrt{5}}{60}[D_1^* + 2(D_{10}^* + D_{11}^* + D_{12}^* + D_{13}^* + D_{14}^* + D_{15}^* + D_{20}^* + D_{21}^* +$$

$$+ D_{22}^* + D_{23}^* + D_{24}^* + D_{25}^* + D_{30}^* + D_{31}^* + D_{32}^* + D_{33}^* + D_{34}^* + D_{35}^*) -$$

$$- 3(D_2^* + D_3^* + D_4^* + D_5^* + D_6^* + D_7^* + D_8^* + D_9^* + D_{16}^* + D_{17}^* + D_{18}^* +$$

$$+ D_{19}^* + D_{26}^* + D_{27}^* + D_{28}^* + D_{29}^*)],$$

$$
\begin{aligned}
\Phi_2^8 = O_{X_1\dots X_4} D_5 = \frac{\sqrt{2}}{48}\,[& 12D_5^* + 9(\bar{D}_1 + \bar{D}_2 + \bar{D}_4) + 6(\bar{D}_6 + \bar{D}_7 + \bar{D}_{10} + D_{16} + D_{17} + \\
& + D_{25} + \bar{D}_{26} + \bar{D}_{27} + \bar{D}_{30}) + 4(D_9^* + D_{12}^* + D_{14}^* + D_{19}^* + D_{21} + D_{23}^* + \\
& + \bar{D}_{24} + D_{29}^* + D_{32}^* + D_{34}^*) - 12D_3^* - 4(D_8 + D_{11} + D_{13} + \bar{D}_{18} + \bar{D}_{22} + \\
& + \bar{D}_{24} + D_{28} + D_{31} + D_{33}) - (\bar{D}_8 + \bar{D}_{11} + \bar{D}_{13} + D_{18} + D_{22} + D_{24} + \\
& + \bar{D}_{28} + \bar{D}_{31} + \bar{D}_{33})],
\end{aligned}
$$

$$
\begin{aligned}
\Phi_3^8 = O_{X_1\dots X_4} D_4 = \frac{\sqrt{6}}{144}\,[& 6D_4^* + 18D_4 + 8(D_{15}^* + D_{20}^* + D_{35}^*) + 4(D_8^* + D_9^* + D_{11}^* + \\
& + D_{12}^* + D_{18}^* + D_{19}^* + D_{23}^* + D_{24}^* + D_{28}^* + D_{29}^* + D_{31}^* + D_{32}^*) + 2(\bar{D}_8 + \\
& + \bar{D}_9 + \bar{D}_{11} + \bar{D}_{12} + D_{18} + D_{19} + D_{23} + D_{24} + \bar{D}_{28} + \bar{D}_{29} + \bar{D}_{31} + \bar{D}_{32}) - \\
& - 18(\bar{D}_1 + \bar{D}_{12}) - 8(D_7^* + D_{10}^* + D_{17}^* + D_{25}^* + D_{27}^* + D_{30}^*) - 6(\bar{D}_7 + \\
& + \bar{D}_{10} + D_{17} + D_{25} + \bar{D}_{27} + \bar{D}_{30}) - 3(D_3^* + D_5^*) - 9(D_3 + D_5) - \\
& - 6(\bar{D}_6 + D_{16} + \bar{D}_{27}) - (D_{13}^* + D_{14}^* + D_{21}^* + D_{22}^* + D_{33}^* + D_{34}^*) - \\
& - 3(D_{13} + D_{14} + \bar{D}_{21} + \bar{D}_{22} + D_{33} + D_{34})],
\end{aligned}
$$

$$
\begin{aligned}
\Phi_4^8 = O_{X_1\dots X_4} D_2 = \frac{\sqrt{3}}{36}\,[& 9D_2^* + 2(D_{13}^* + D_{14}^* + D_{15}^* + D_{20}^* + D_{21}^* + D_{22}^* + D_{33}^* + D_{34}^* + \\
& + D_{35}^*) + (D_7^* + D_8^* + D_9^* + D_{17}^* + D_{18}^* + D_{19}^* + D_{27}^* + D_{28}^* + D_{29}^*) - \\
& - 3(D_3^* + D_4^* + D_5^* + D_6^* + D_{16}^* + D_{26}^*) - 2(D_{10}^* + D_{11}^* + D_{12}^* + D_{23}^* + \\
& + D_{24}^* + D_{25}^* + D_{30}^* + D_{31}^* + D_{32}^*)],
\end{aligned}
$$

$$
\begin{aligned}
\Phi_5^8 = O_{X_1\dots X_4} D_{10} = \frac{1}{12}\,[& 16(\bar{D}_{11} + \bar{D}_{12}) + (\bar{D}_{13} + \bar{D}_{14} + \bar{D}_{20} + D_{25} + \bar{D}_{30} + D_{35}) + \\
& + 8(\bar{D}_2 + \bar{D}_4) + 6(\bar{D}_3 + \bar{D}_5 + \bar{D}_8 + \bar{D}_9 + D_{18} + D_{19} + \bar{D}_{28} + \bar{D}_{29}) + \\
& + 4(D_{10}^* + D_{15}^*) - 2D_{15} + D_{21}^* + D_{22}^* + D_{23}^* + D_{24}^* + D_{31}^* + D_{32}^* + D_{33}^* + \\
& + D_{34}^* - 2(\bar{D}_1 + D_{11} + D_{12} + D_{13} + D_{14} + D_{16} + D_{17} + D_{20} + \bar{D}_{25} + \\
& + \bar{D}_{26} + \bar{D}_{27} + D_{30} + \bar{D}_{35})],
\end{aligned}
$$

$$
\begin{aligned}
\Phi_6^8 = O_{X_1\dots X_6} D_{11} = \frac{\sqrt{3}}{24}\,[& 8(D_{14} + D_{19} + \bar{D}_{28} + \bar{D}_{29}) + 4(D_{11} + D_{13} + \bar{D}_{14} + D_{17}) + \\
& + 3(\bar{D}_3 + \bar{D}_9 + \bar{D}_{27}) + 2(D_{22}^* + D_{23}^* + D_{32}^* + D_{33}^*) + \bar{D}_{11} + \bar{D}_{12} - \\
& - 6(\bar{D}_1 + \bar{D}_2 + \bar{D}_6) - 4(D_{12} + \bar{D}_{13}) - 3(\bar{D}_5 + \bar{D}_8) - 2(D_{21}^* + D_{24}^* + \\
& + D_{31}^* + D_{34}^*)],
\end{aligned}
$$

$$\Phi_7^8 = O_{X_1 \ldots X_4} D_6 = \frac{\sqrt{6}}{432} [72 D_6^* + 24(D_{13} + D_{14} + D_{15}^* + \bar{D}_{25}) + 12(\bar{D}_{13} + \bar{D}_{14} + D_{17}^* +$$
$$+ D_{18}^* + D_{19}^* + D_{23}^* + D_{24}^* + D_{25} + D_{27}^* + D_{28} + D_{29} + D_{30}^* + D_{31} + D_{32}) +$$
$$+ 9(\bar{D}_{31} + \bar{D}_{32}) + 6(\bar{D}_4 + \bar{D}_{28} + \bar{D}_{29}) - 36(D_{16}^* + D_{26}) - 28\bar{D}_{26} -$$
$$- 24(D_7 + D_8^* + D_9^* + D_{10} + D_{11} + D_{12}) - 21(\bar{D}_{11} + \bar{D}_{12}) -$$
$$- 18(\bar{D}_7 + \bar{D}_{10} - 15(\bar{D}_{21} + \bar{D}_{22}) - 12(D_{20}^* + D_{21} + D_{22} + D_{33}^* +$$
$$+ D_{34}^* + D_{35}) - 4\bar{D}_2],$$

$$\Phi_8^8 = O_{X_1 \ldots X_6} D_8 = \frac{\sqrt{6}}{36} [32\bar{D}_8 + 14(D_{19} + \bar{D}_{29}) + 12\bar{D}_{13} + 4D_8 + 2(D_{12}^* + D_{14}^* + \bar{D}_{19} +$$
$$+ D_{29}) + D_{22}^* + D_{24}^* + \bar{D}_{31}^* + D_{33}^* - 36\bar{D}_1 - 14(\bar{D}_{18} + \bar{D}_{28}) - 12(\bar{D}_2 +$$
$$+ \bar{D}_4 + \bar{D}_5 + D_{16} + D_{17} + D_{26} + \bar{D}_{27}) - 4D_9^* - 2(D_{12} + D_{13} + D_{15} +$$
$$+ \bar{D}_{18} + D_{28}) - (\bar{D}_{11} + \bar{D}_{13} + D_{21}^* + D_{23}^* + D_{32}^* + D_{34}^*)],$$

$$\Phi_9^8 = O_{X_1 \ldots X_6} D_7 = \frac{\sqrt{3}}{36} [8D_7^* - 2\bar{D}_7 + 4(D_{15}^* + \bar{D}_{18} + \bar{D}_{19} + D_{28} + D_{29}) + 2(D_{11}^* + D_{12}^* +$$
$$+ D_{18} + D_{19} + D_{20} + D_{25}^* + \bar{D}_{28} + \bar{D}_{29} + D_{30} + \bar{D}_{35}) + \bar{D}_3 + \bar{D}_5 + D_{21} +$$
$$+ D_{22} + \bar{D}_{30} + \bar{D}_{33} + \bar{D}_{34} - 5\bar{D}_{10} - 3(\bar{D}_6 + \bar{D}_8 + \bar{D}_9 - 4(D_8 + D_9 +$$
$$+ D_{10} + D_{13} + D_{14} + D_{17}^* + D_{20} + D_{27}^* + \bar{D}_{35}) - 2(\bar{D}_1 + \bar{D}_2 + \bar{D}_4 + \bar{D}_{13} +$$
$$+ \bar{D}_{14} + \bar{D}_{20} + D_{23}^* + D_{24}^* + D_{31}^* + D_{32}^* + D_{35}) - \bar{D}_{26}],$$

$$\Phi_{10}^8 = O_{X_1 \ldots X_4} D_{26} = \frac{\sqrt{2}}{12} [3D_{26}^* + D_{17}^* + D_{18}^* + D_{19}^* + D_{23}^* + D_{24}^* + D_{25}^* + D_{33}^* + D_{34}^* + D_{35}^* -$$
$$- 3D_{16}^* - (D_{20}^* + D_{21}^* + D_{22}^* + D_{27}^* + D_{28}^* + D_{29}^* + D_{30}^* + D_{31}^* + D_{32}^*)],$$

$$\Phi_{11}^8 = O_{X_1 \ldots X_6} D_{28} = \frac{\sqrt{3}}{12} [4(\bar{D}_3 + \bar{D}_9) + 2(D_{19}^* + D_{22} + D_{28} + \bar{D}_{29} + D_{32}) + (\bar{D}_{11} + \bar{D}_{22} +$$
$$+ \bar{D}_{24} + \bar{D}_{32} + \bar{D}_{34} - 14\bar{D}_1 - 6(\bar{D}_2 + \bar{D}_4 + \bar{D}_6) - 4(\bar{D}_5 + \bar{D}_8 + \bar{D}_{26} + \bar{D}_{27}) -$$
$$- 2(\bar{D}_7 + D_{16} + D_{18}^* + \bar{D}_{28} + D_{29}) - (\bar{D}_{13} + D_{21}^* + D_{23}^* + D_{31}^* + D_{33}^*)],$$

$$\Phi_{12}^8 = O_{X_1 \ldots X_6} D_{27} = \frac{1}{2} [4(\bar{D}_{26} + D_{27}^*) + 2(D_{18} + D_{19} + \bar{D}_{20} + \bar{D}_{25} + \bar{D}_{30} + \bar{D}_{35}) + D_{21} +$$
$$+ D_{22} + D_{23} + D_{24} + D_{31} + D_{32} + D_{33} + D_{34} - 4(D_{16} + D_{17}^*) -$$
$$- 2(D_{20} + D_{25} + \bar{D}_{28} + \bar{D}_{29} + D_{30} + D_{35}) - (\bar{D}_{21} + \bar{D}_{22} + \bar{D}_{23} + \bar{D}_{24} +$$
$$+ \bar{D}_{31} + \bar{D}_{32} + \bar{D}_{33} + \bar{D}_{34})],$$

$$\Phi_{13}^8 = O_{X_1 \dots X_8} D_{30} = \frac{\sqrt{3}}{24} [4(D_{30} + D_{35}^*) + 2(D_{21}^* + D_{22}^* + D_{23}^* + D_{24}^*) + \bar{D}_{30} -$$

$$- 4(D_{20}^* + \bar{D}_{25}) - 2(D_{31}^* + D_{32}^* + D_{33}^* + D_{34}^*) - D_{25}],$$

$$\Phi_{14}^8 = O_{X_1 \dots X_8} D_{31} = \frac{1}{4} [D_{22}^* + D_{23}^* + D_{31} - 2\bar{D}_5 - (\bar{D}_{11} + D_{18} + D_{21}^* + D_{24}^* + \bar{D}_{28} +$$

$$+ D_{32}^* + D_{33}^* + \bar{D}_{34})].$$

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n-ЕЛЕКТРОН (n=2, 4, 6‘ 8) СИНГЛЕТЫ КАК СОБСТВЕННЫЕ ФУНКЦИИ S^2

Ф. Беренц

n-електрон (n=2, 4, 6, 8) синглеты, как собственные функции S^2 были получены методом спиновых операторов.